



chain nodes :

19 20 21 22 23 25 26 27 33 34 35 36 37

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 24 28 29 30 31 32

chain bonds :

6-19 7-20 14-22 19-20 20-21 21-33 21-34 22-23 22-35 23-24 23-25 25-26 25-27 34-35  
35-37 35-36

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16  
16-17 17-18 24-28 24-32 28-29 29-30 30-31 31-32

exact/norm bonds :

21-33 21-34 25-26 25-27 34-35

exact bonds :

6-19 7-20 14-22 19-20 20-21 22-23 22-35 23-24 23-25 35-37 35-36

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15 15-16  
16-17 17-18 24-28 24-32 28-29 29-30 30-31 31-32

G1:MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,PhO,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:Atom 29:Atom 30:Atom 31:Atom  
32:Atom 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS